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Direct Experimental Evidence for Reactions between Dissolved Acid Halide and Chlorine Nitrate

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Cluster chemistry employing a fast flow reactor was used to evaluate the enhanced reactivity of chlorine nitrate ($ClONO_2$) with dissolved acid halide. Reactions of $ClONO_2$ with deuterium chloride doped deuterated water clusters $[D^+(D_2O)_m(DCl)_n$, ($m = 10-14$, $n = 1,2$)] were investigated under thermal conditions over a temperature range of 148−158 K; deuterated species were employed in place of light hydrogen containing molecules to facilitate the determination of reaction mechanisms. Chemical reactions were found to occur between water clusters and chlorine nitrate only under conditions where dissolved deuterium chloride was present. Nitric acid is found to remain within the water cluster to yield gaseous chlorine (Cl_2) from the water cluster. These results provide direct evidence that an ionic reaction mechanism is involved in the heterogeneous reaction of hydrogen chloride and chlorine nitrate on clusters that mimic polar stratospheric cloud surfaces.

Introduction

There has been extensive interest in the annual depletion of stratospheric ozone over the Antarctic since its reported discovery in 1985.[1] Heterogeneous reactions on polar stratospheric clouds (PSCs) have been suggested as a significant contributor in the catalytic destruction of reservoir species such as HCl and $ClONO_2$.[2] In the case of the chemical transformation of $ClONO_2$ to HNO_3, two mechanisms have been suggested to occur on PSCs:

$$H_2O + ClONO_2 \rightarrow HNO_3 + HOCl \tag{1}$$

$$HCl + ClONO_2 \rightarrow HNO_3 + Cl_2 \tag{2}$$

Much theoretical and experimental effort has been invested in understanding the reaction mechanisms that are involved in reactions 1 and 2, but an understanding of the microphysical properties at the surface of polar stratospheric cloud (PSCs) particles is still lacking.[3] The hydrolysis of $ClONO_2$ has been studied extensively by many experimental and theoretical groups.[4−6] An acid catalysis mechanism was proposed by Wofsy et al.[7] for the heterogeneous hydrolysis of $ClONO_2$ by the following process:

$$ClONO_2 + H^+ \rightarrow Cl^{+-}HNO_3 \tag{3}$$

Recent studies by Horn and co-workers have suggested an S_N2-type reaction mechanism for reaction 1 where H_2O attacks the Cl atom of $ClONO_2$ to form a reactive intermediate $[H_2OCl^+]$,[8] as follows:

$$H_2O + ClONO_2 \rightarrow [H_2OCl]^+ + NO_3^- \tag{4}$$

On the basis of electronic structure calculations, Hynes et al.[6] have proposed a different hydrolysis scheme than reaction 4. A nucleophilic attack of a water molecule on the chlorine atom of $ClONO_2$, followed by a proton transfer between the attacking water molecule and the surrounding ice lattice, was proposed by Hynes et al. A proton-transfer mechanism allows for the water molecule to become a stronger nucleophile (OH^-). These theoretical calculations suggest a fast reaction between water and $ClONO_2$, which is consistent with experimental observations. Several gas-phase studies of water cluster ions and $ClONO_2$ have been investigated.[9−15] Although reactions between protonated water clusters $[H^+(H_2O)_n]$ and $ClONO_2$ have been reported to occur,[13,15] Viggiano and co-workers found negligible reactivity between $ClONO_2$ and protonated water cluster for cluster sizes (n) greater than 1 at thermal conditions. Recently, we have extended the Viggiano experiments by exploring reactions of protonated water clusters as a function of cluster size and also failed to observe chemical reactions at thermal conditions.[16] It is possible that the reactions observed by Bondybey and Okumura experiments could have been influenced by limitations of their experimental techniques.

On the other hand, evidence clearly exists for reactions of $ClONO_2$ and HCl on ice surfaces to occur by an ionic mechanism. An ionic solvation mechanism has been invoked to account for the fact that reaction 2 is extremely slow in the gas phase, but very rapid on ice surfaces.[17,18] Theoretical and experimental results have suggested the first step in reaction 2 is the dissolution of HCl, resulting in the solvation of its ion pairs.[19,20] Using high-level electronic structure calculations, Hillier and co-workers have found the reaction of HCl and $ClONO_2$ to proceed initially by the ionization of HCl to generate the Cl^- nucleophile.[21] Employing a quantum mechanical approach, Bianco and Hynes studied reaction 2 on a model ice lattice and reported a reaction mechanism involving a nucleophilic attack of Cl^- on the electrophilic chlorine atom in $ClONO_2$.[22] Xu and co-workers have theoretically investigated the reaction of $ClONO_2$ with HCl on water clusters and found reactions to proceed faster as the cluster size increases due to an enhancement of the ionic character of the chemical species involved through hydration.[23]

Molina and co-workers have investigated reaction 2 on

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various ice surfaces and have obtained results that are consistent with an ionic reaction mechanism involving HCl solvation on liquidlike surface layer,[24] whereupon the chloride ion from dissolved hydrogen chloride is envisioned to attack the chlorine atom of chlorine nitrate. Using infrared spectroscopy in conjunction with thermal desorption mass spectrometry, Horn and co-workers provided evidence for a heterogeneous reaction of Cl^- with $ClONO_2$ under stratospheric conditions.[25] Vickerman and co-workers using static secondary ion mass spectrometry have studied water ice films, to simulate type II polar stratospheric cloud (PSC) particles, exposed to various concentrations of HCl. HCl was found to rapidly dissociated to form solvated ions.[26] There was no evidence for the adsorption of intact molecular HCl. The interactions of $ClONO_2$ and HCl with ice films was probed using static secondary ion mass spectrometry.[27] Vickerman and co-workers found $ClONO_2$ to react directly in the presence of a solvated Cl^- nucleophile to form molecular chlorine and solvated nitric acid. Shultz and co-workers support the role of ionic mechanisms for HCl on heterogeneous aerosol surfaces and obtained experimental evidence for the ionization of HCl on ice surfaces representative of heterogeneous stratospheric surfaces.[28,29] Using sum frequency generation spectroscopy, HCl was found to dissociate and form highly hydrated species, and molecular HCl was not found to be absorbed on these water surfaces.

Previous research from other research groups and ours have found compelling evidence for the dissolution of various acid species by water clusters. Kay et al. formed $D_3O^+(DNO_3)(D_2O)_n$ ($n = 1-12$) by ionizing neutral clusters of nitric acid and water in molecular beam.[30] A minimum in the cluster size distribution at $n = 4$ was reported. This abrupt minima at $n = 4$ was explained as the formation of solvated ion pairs. Interestingly, Zhang et al. probed the reactions of $D_3O^+(D_2O)_n$ with DNO_3 using a variable-temperature fast flow reactor. The uptake of nitric acid by protonated water clusters was observed to occur at $n > 4$.[31] The first uptake found by Zhang et al. is the same as the first point of dissolution of nitric acid by water clusters reported by Kay et al. Dissolved acid species (HCl, HNO_3, HBr) within a water cluster were found to be responsible for an enhanced association of an additional acid species due to the availability of an active coordinate sites (Cl^-, NO_3^-, Br^-).[32,33] The Bondybey research group has also investigated dissolution/precipitation reactions of HCl in water clusters using a Fourier transform cyclotron resonance apparatus[34−36] and obtained similar results and conclusions as our research group. Clary and co-workers used ab initio MP2 equilibrium geometries of clusters of $HCl(H_2O)_n$ ($n = 1-3$) and concluded that HCl ionizes when the cluster size is greater than 3.[37]

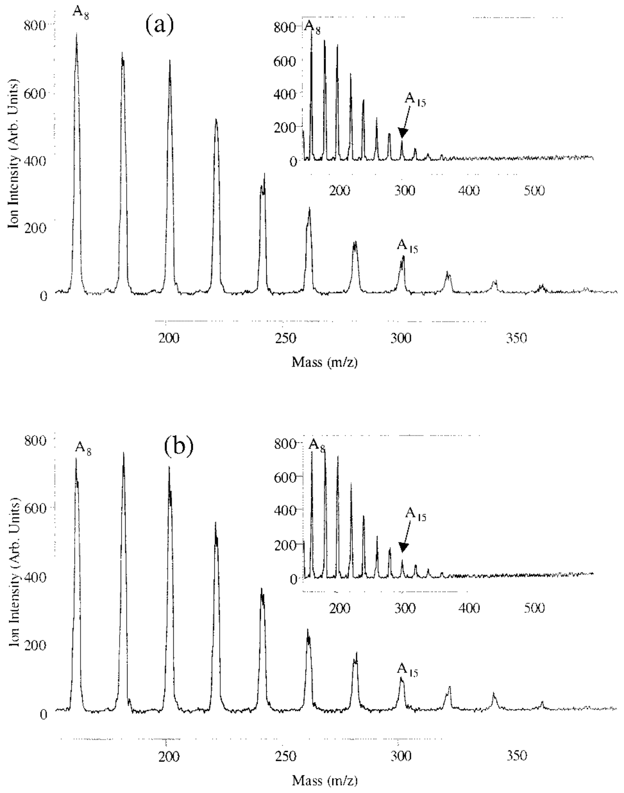

Figure 1. Mass spectra of $D^+(D_2O)_n$ obtained before (a) and after (b) the addition of 1.23×10^{12} cm^{-3} $ClONO_2$. Pressure: 0.3 Torr; temperature: 154 K. $A_n = D^+(D_2O)_n$. Note the similarities establishing that no reaction occurs.

Experiment Section

To fully elucidate the proposed ion-solvated mechanism of reaction 2, we undertook studies of the reaction employing clusters of known composition using a fast-flow reactor affixed with a high-pressure ion source. The details of this apparatus and experimental procedure have been described in previous publications[38−41] and only a brief outline pertinent to experiments in this paper is given here. In the ion source, water cluster ions are generated by the discharge ionization of a D_2O/helium mixture. Deuterium chloride was added into the source by a separate inlet to generate mixed deuterium chloride water cluster ions. The employment of heavy water (D_2O) and heavy hydrogen chloride (DCl) is critical in the determination of the reaction mechanisms of $ClONO_2$ with water cluster ions. Water cluster ions are carried into the flow tube by a continuous flow of 7000 sccm (standard cubic centimeter per minute) of helium buffer gas which is maintained at a selected monitored pressure (0.3 Torr). A selected concentration of $ClONO_2$ reactant gas is introduced approximately 30 cm downstream of the source. Reactant and product ions are sampled, scanned by a quadrupole mass spectrometer, and detected by a channeltron electron multiplier. The flow-tube and helium buffer gas temperatures ranged from 148 to 158 K, and was controlled with an accuracy of ±1 K. The $ClONO_2$ sample used in these experiments was synthesized based on the method of Schmeisser.[42] The rate coefficient of I^- with $ClONO_2$ is known, and we employed this value in combination with the rate measurements made in our laboratory to deduce the actual concentration of $ClONO_2$ prepared in our studies.[43] This procedure is necessary since it is known that HNO_3 can be a major impurity in the synthesis method. The rate coefficient of I^- with $ClONO_2$ observed in our experiment is determined to be $0.62 \pm 27\% \times 10^9$ cm^3 s^{-1}. Huey and co-workers measured the rate coefficient of I^- and $ClONO_2$ and report the rate coefficient to be $0.90 \pm 40\% \times 10^{-9}$ cm^3 s^{-1}.[10] The experimental determined rate coefficient compares well with the calculated rate coefficient of 0.96×10^{-9} cm^3 s^{-1}, determined on the basis of Su−Chesnavich theory[44,45] and with previous experiments. NO_3^- is the primary product ion formed from the reaction of I^- and $ClONO_2$. $NO_3^-(ClONO_2)$ secondary product ions was observed, and $NO_3^-(HNO_3)$ secondary product ions were not observed. A Cl_2 impurity from the Cl_2O synthesis was not detected in these I^- and $ClONO_2$ experiments. These studies indicate very little HNO_3 and Cl_2 impurities are present in the $ClONO_2$ sample prepared. The $ClONO_2$ sample employed in this experiment is about 65% pure based on the measured rate coefficient and calculated rate coefficient.

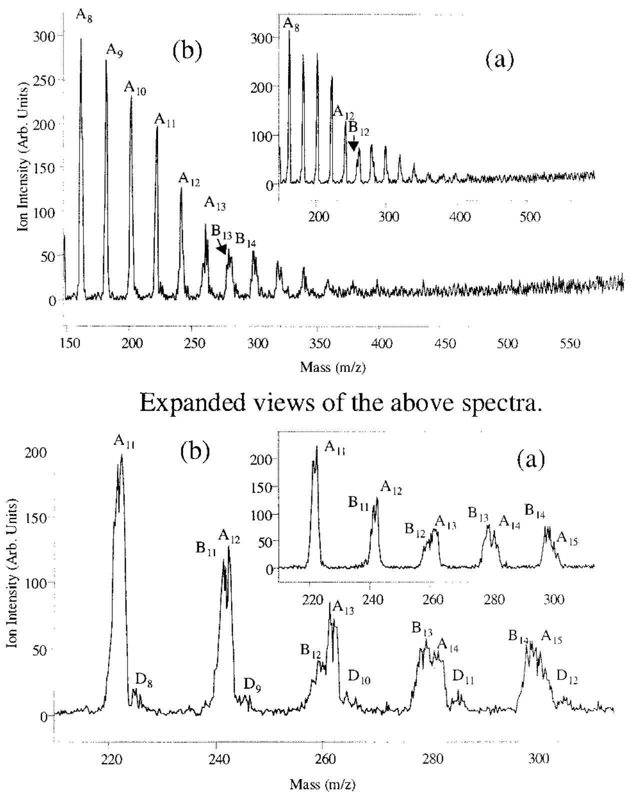

Figure 2. Mass spectra of $D^+(D_2O)_n(DCl)$ obtained before (a) and after (b) the addition of 1.23×10^{12} cm^{-3} $ClONO_2$. Pressure: 0.3 Torr; temperature: 154 K. $A_n = D^+(D_2O)_n$; $B_n = D^+(D_2O)_n(DCl)$; $D_n = D^+(D_2O)_n(DNO_3)$. The product ions, D_n, from reactions of $ClONO_2$ with dissolved deuterium chloride are clearly discernible.

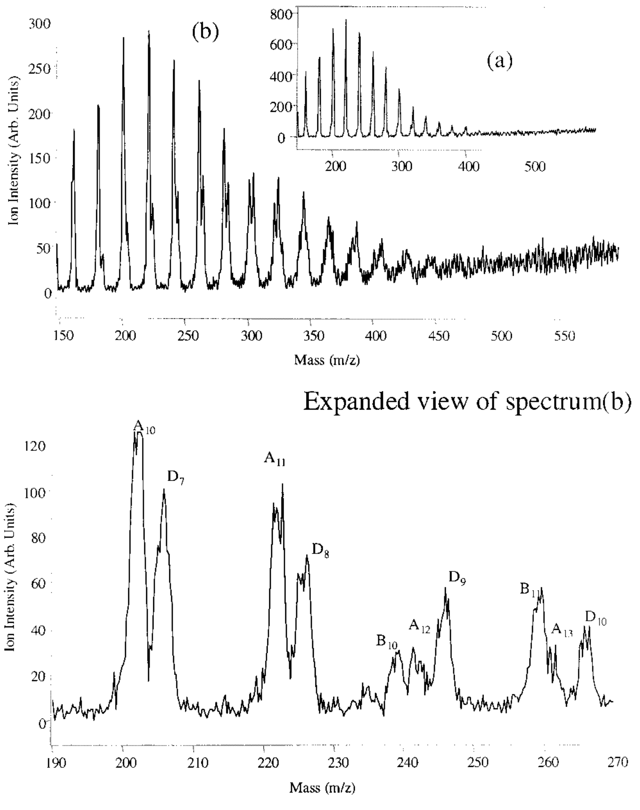

Figure 3. Mass spectra of $D^+(D_2O)_n(DCl)$ obtained before (a) and after (b) the addition of 3.62×10^{12} cm^{-3} $ClONO_2$. Pressure: 0.3 Torr; temperature: 151 K. $A_n = D^+(D_2O)_n$; $B_n = D^+(D_2O)_n(DCl)$; $D_n = D^+(D_2O)_n(DNO_3)$.

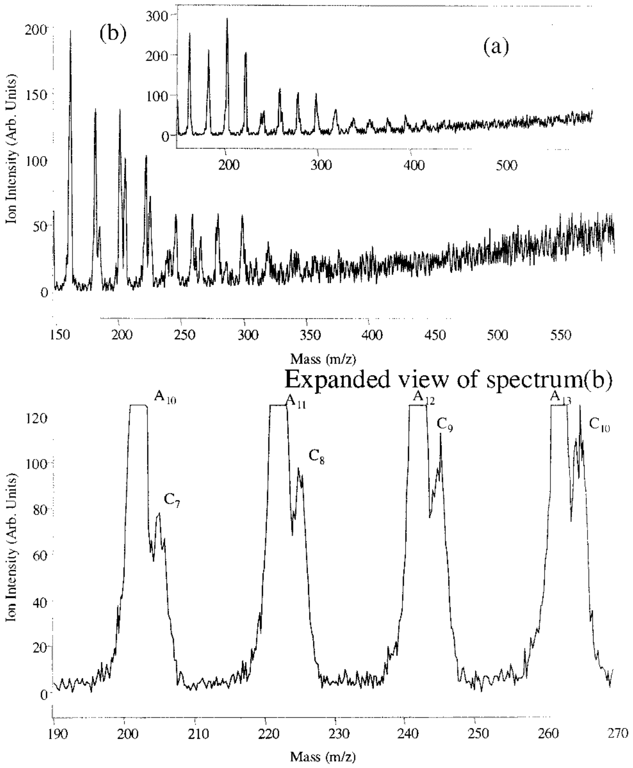

Figure 4. Mass spectra of $D^+(D_2O)_n$ obtained after the addition of 1.91×10^{12} cm^{-3} HNO_3. Pressure: 0.3 Torr; temperature: 151 K. $A_n = D^+(D_2O)_n$; $C_n = D^+(D_2O)_n(HNO_3)$.

Results and Discussion

As a first step, experiments were conducted to investigate whether reactions occur between $D_3O^+(D_2O)_n$ ($n = 7-16$) and $ClONO_2$ under thermal conditions; no chemical reactions were observed to occur. See Figure 1. Figure 1a shows a typical distribution of protonated water cluster before the addition of 1.23×10^{12} cm^{-3} $ClONO_2$. After the addition of $ClONO_2$ (Figure 1b), the ion intensity of protonated water clusters did not decrease and the formation of DNO_3 reaction product ions did not occur. These results are consistent with previous work from our research group[41] which served to explain several conflicting observations of the reactivity of water clusters and $ClONO_2$.[13-15] An acid-catalyzed mechanism is not supported by these results and is not expected to be involved in the conversion of $ClONO_2$ to HNO_3 on polar stratospheric cloud surfaces as had previously been suggested. Moreover, reactions between the waters of hydrations and $ClONO_2$ were too slow to be observed under chosen experimental conditions.

In the next series of experiments, DCl was used to dope deuterated protonated water clusters. These subsequent studies were conducted at a similar temperature, pressure, and helium flow as the experiments completed in Figure 1 and revealed that reactions *do occur* between the reactant ions containing DCl and $ClONO_2$. See Figure 2. Water cluster ions containing DCl (B_n) appeared 3 amu less than the protonated water clusters. Product ions of the form $D^+(D_2O)_n(DNO_3)$ (D_n) appeared at $n = 8$. Product ions (D_n) from reactions of $ClONO_2$ with dissolved deuterium chloride are clearly visible and contain DNO_3. A reaction mechanism has been proposed to occur between the hydrated chloride anions and chlorine nitrate:[9]

$$Cl^-(D_2O)_n + ClONO_2 \rightarrow [(D_2O)_nCl^- \cdots ClONO_2]^* \rightarrow NO_3^-(D_2O)_m + Cl_2 + (n-m)D_2O \quad (5)$$

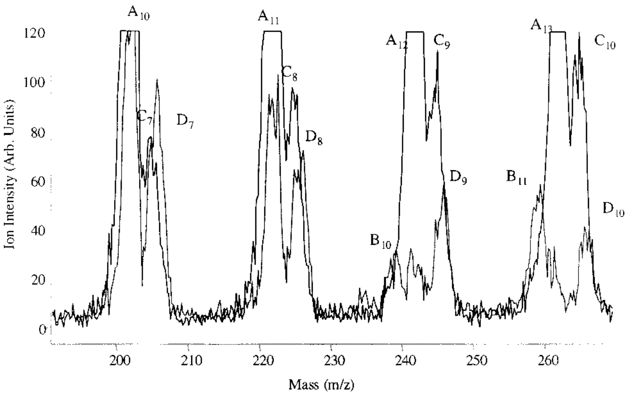

Figure 5. Expanded views of Figures 3b and 4b. Notice the mass difference between nitric acid product ions from nitric acid and ClONO$_2$ (C$_n$ and D$_n$).

Since deuterium chloride dissolves within the water cluster, the product ions observed could be formed by the following reaction mechanism:

$$\mathrm{D^+(D_2O)_n(DCl)}\ [\leftrightarrow \mathrm{D^+(D_2O)_xD^+(D_2O)_yCl^-(D_2O)_z}] + \mathrm{ClONO_2} \rightarrow \mathrm{D^+(D_2O)_p(DNO_3)} \leftrightarrow [\mathrm{D^+(D_2O)_xD^+(D_2O)_yNO_3^-(D_2O)_m}] + \mathrm{Cl_2} + (z-m)\mathrm{D_2O} \qquad (n = x + y + z;\ p = x + y + m) \quad (6)$$

As determined by thermodynamic information,[46−49] reaction 5 is exothermic for $(n - m) \leq 2$ and therefore reaction 6 is also expected to be exothermic and water molecules are expected to evaporate from the product cluster ion. From these experiments, we believe DNO$_3$ product ions ($D_{n\geq8}$ from Figure 2) are from reactions with DCl-doped water clusters ($B_{n\geq11}$ from Figure 2).

To accurately determine product ions generated when ClONO$_2$ reacted with DCl-doped water clusters, a dilution of HNO$_3$ was prepared in a second separate mixing chamber and added to the flow tube to a distribution of protonated water clusters under similar conditions as the dissolved DCl and ClONO$_2$ experiments. See Figures 3 and 4. The product ions formed from reactions with HNO$_3$ ($C_{n\geq7}$) were compared to the product ions of ClONO$_2$ ($D_{n\geq7}$) and were found to be different by 1 amu for the first uptake of nitric acid. See Figure 5. Reaction product ions from ClONO$_2$ ($D_{n\geq7}$) are from reactions with DCl-doped water clusters ($B_{n\geq10}$) as determined from available thermodynamic information.

To further address the issue of reactivity of dissolved deuterium chloride, experiments were performed with ClONO$_2$ in which the first and second uptake of DCl by protonated water clusters was present. These experiments are presented in Figure 6. Figure 6 provides evidence for the observed reaction product ions contained DNO$_3$ by the formation of $\mathrm{D^+(D_2O)_n(DCl)(DNO_3)}$ cluster ions.

Conclusions

The reactivity of dissolved deuterium chloride water clusters to ClONO$_2$ compared to protonated water clusters as found in the present study clearly demonstrates the reactivity of the solvated chloride ions to ClONO$_2$. This observation strongly suggests the reactivation of ClONO$_2$ on PSCs with HCl species will proceed by an ionic solvation mechanism as opposed to a mechanism involving intact molecular HCl. Based on our results of protonated water clusters and ClONO$_2$, an acid catalysis mechanism is not expected to be involved in the hydrolysis of ClONO$_2$. The waters of hydration in these experiments were not sufficient to reduce the barrier for reactions between protonated water clusters and ClONO$_2$. These results would suggest that the role of water is to aid in the dissociation of ClONO$_2$. It is recognized that water clusters are not exact replicates of cloud surfaces, but the spirit of our work is to provide detailed insights into the solvation and reactivity of ion pairs. The findings reported herein provide complementary information pertaining to potential reaction mechanisms which have been suggested to occur on cloud surfaces. In future studies, the reactivity of other solvated acid molecules such as nitric acid toward ClONO$_2$ and N$_2$O$_5$ will be investigated and

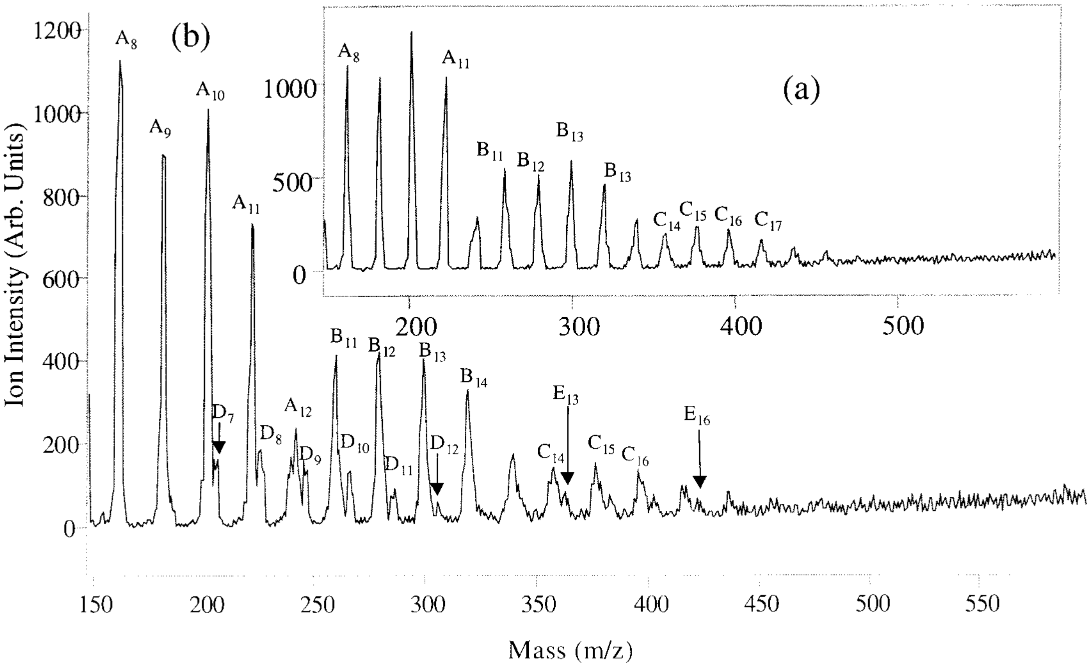

Figure 6. Mass spectra of $\mathrm{D^+(D_2O)_n(DCl)}$ obtained before (a) and after (b) the addition of 3.13×10^{12} cm^{-3} ClONO$_2$. Pressure: 0.3 Torr; temperature: 151 K. $A_n = \mathrm{D^+(D_2O)_n}$; $B_n = \mathrm{D^+(D_2O)_n(DCl)}$; $C_n = \mathrm{D^+(D_2O)_n(DCl)_2}$; $D_n = \mathrm{D^+(D_2O)_n(DNO_3)}$; $E_n = \mathrm{D^+(D_2O)_n(DNO_3)(DCl)}$.

probed since nitric acid is an important constituent of type I polar stratospheric clouds.

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